L01: Desktop Molecular Graphics PyMol 1

From the preface of the User's guide: "*PyMOL was created in an efficient but highly pragmatic manner, with heavy emphasis on delivering powerful features to end users. Expediency has almost always taken precedence over elegance, and adherence to established software development practices is inconsistent. PyMOL is about getting the job done now, as fast as possible, by whatever means were available.*"
PyMol is a multiplatform molecular graphics software with many advanced features such as rendered cartoon ribbons and surfaces, internal ray tracing and movie tools and is fast becoming the new "standard" in molecular graphics. The PyMol web site is located at http://pymol.sourceforge.net/

Biochemistry students can download the latest PyMol version from a campus network at http://www.biochem.wisc.edu/it/resources.aspx

Note: within the exercises, **Bold** text shows what actions are taken by the user : typing text or clicking the mouse.

Whenever possible a "call for action" icon (√ or ✔) will be shown.

1 *PyMol - Exercise A*: Download a PDB from the repository

Reminder: Structures have a PDB ID code made of 4 letters and numbers. PDB files contain coordinates pertinent to the crystallographic arrangement of the molecules within the crystal. The biological functional entity can be either a multimer of the deposited structure, or just one of multiple copies within the file. In the following example we will download one functional biological subunit, in this case a monomer.

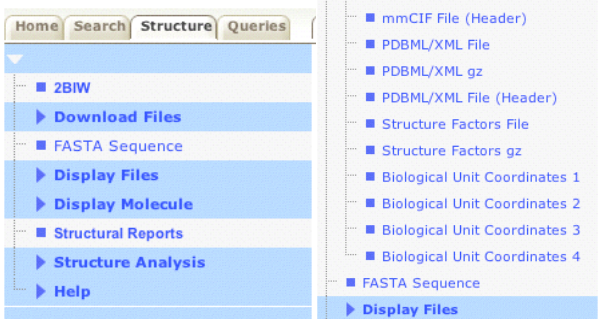
✔ **TASK**

- **Open a web browser** such as Safari or Firefox.
- Point your web browser to **`www.rcsb.org`**
- In the Search box enter the following ID: **2biw** and **click SEARCH button**

- On the left column click **Download Files** to show submenus
- **Click** the first option **Biological UnitCoordinates 2**

Note: DO NOT USE Biological Unit Coordinates 1

- The file is saved on the desktop as **2BIW.pdb2**



Note: The file might be delivered as a gunzipped (.gz) file. However the browser should decode it automatically.

You can now close your browser, or hide it (Command-H).

Optional exercise: explore the *text* content of the PDB file 2BIW.pdb2

You can review details on the PDB file format in the previous section titled "Desktop molecular graphics: background essentials" and online at http://www.rcsb.org (On the left menu table click on "Dictionaries & File Formats" and select "PDB format."

In summary, PDB files are the simplest plain text files organized in column format in lines of at most 80 characters. Each line (record) starts with a keyword. The top of the file (header) contains informative records, while ATOM and HETATM records represent the 3D coordinates.

Open 2BIW.pdb2 with a simple word processor (the simpler the better! For example "TextEdit on a Macintosh or "Wordpad" in Windows. Windows simple "Notepad" usually does not work because it does not translate end-of-line characters.

Scroll up and down the text file and observe the contents.

Since we only saved a portion of the original PDB data by selecting a biological unit monomer, the header is somewhat shorter (428 lines before the first ATOM record) than if we had saved the complete PDB file (998 lines; you can download the complete 2BIW.pdb file if you wish.) Note that within the 2BIW.pdb2 header, the XXXX next to the release date on the first line are replacing the `2BIW` PDB ID code as 2BIW.pdb2 does not represent the complete PDB records.

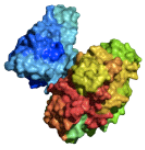
```
HEADER    OXIDOREDUCTASE                          19-JAN-05   XXXX
TITLE     CRYSTAL STRUCTURE OF APOCAROTENOID CLEAVAGE OXYGENASE FROM
TITLE    2 SYNECHOCYSTIS, NATIVE ENZYME
COMPND    APOCAROTENOID-CLEAVING OXYGENASE
KEYWDS    OXYGENASE,NON-HEME IRON,CAROTENOID CLEAVAGE,RETINAL
KEYWDS   2 FORMATION, OXIDOREDUCTASE, DIOXYGENASE
EXPDTA    X-RAY DIFFRACTION
AUTHOR    D.P.KLOER, S.RUCH, S.AL-BABILI, P.BEYER, G.E.SCHULZ
JRNL        AUTH   D.P.KLOER, S.RUCH, S.AL-BABILI, P.BEYER, G.E.SCHULZ
JRNL        TITL   THE STRUCTURE OF A RETINAL-FORMING CAROTENOID
JRNL        TITL 2 OXYGENASE
JRNL        REF    SCIENCE                       V. 308   267 2005
JRNL        REFN   ASTM SCIEAS  US ISSN 0036-8075
REMARK   1
SEQRES   1 A  490  MET VAL THR SER PRO PRO THR SER SER PRO SER GLN ARG
SEQRES   2 A  490  SER TYR SER PRO GLN ASP TRP LEU ARG GLY TYR GLN SER
[. . . . . ]
MTRIX2   3 -0.756169  0.514705 -0.404088       13.98510    1
MTRIX3   3  0.610627  0.777006 -0.152957      118.86930    1
ATOM      1  N   GLN B  12      16.794 -17.939  28.900  1.00 71.25           N
ATOM      2  CA  GLN B  12      16.091 -17.967  30.218  1.00 71.00           C
ATOM      3  C   GLN B  12      16.877 -17.181  31.273  1.00 69.76           C
[. . . . . ]
ATOM   3766  CG2 THR B 490      47.002  -0.207  59.451  1.00 73.42           C
ATOM   3767  O'' THR B 490      48.633   0.228  56.341  1.00 73.10           O
TER    3768      THR B 490
HETATM 3769 FE    FE B1492      30.259   6.403  38.822  1.00 45.64          FE
HETATM 3770  O1   3ON B1491      26.391  21.062  36.210  1.00100.47           O
HETATM 3771  C5   3ON B1491      25.099  20.591  36.637  1.00100.23           C
[. . . . . ]
CONECT 3799 3798
CONECT 3800 3798 3801
CONECT 3801 3800
MASTER        0    0    0   36  154    0   24   1515742    4   37  152
END
```

H E A D E R

3 D - D A T A

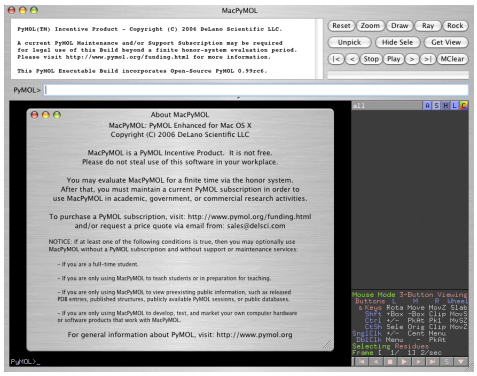
E N D

2 *PyMol - Exercise B*: Open PyMol and load PDB file



PyMol or MacPyMol should be located within **Applications > Classes** on the DMC computer. Your instructor may give you a different location if necessary.

✔ TASK



- double-click on the PyMol icon to launch the software.

Note: Some versions of PyMol have the top and bottom panels in separate windows, but offer the same interface.

- Type the next commands after **PyMOL>** within the *top* line command:

✔ TASK

PyMOL> **cd desktop** Note the echo on the text area above

PyMOL> **pwd** this will echo `/Users/DMC/Desktop` or a similar path. On a Windows system the path would begin with C:\

Note: PyMol uses many Unix commands
cd = change directory
pwd = present working directory

PyMOL> **load 2BIW.pdb2**

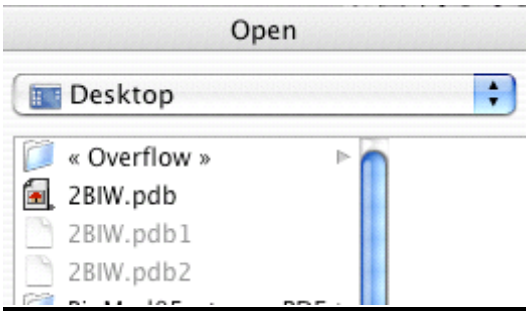
This will load the structure and echo information in the text panel as reproduced to the right.

Note: file name is case sensitive!

```
PyMOL>load 2BIW.pdb2
HEADER    OXIDOREDUCTASE                          19-JAN-05
XXXX
TITLE     CRYSTAL STRUCTURE OF APOCAROTENOID
CLEAVAGE OXYGENASE FROM
TITLE    2 SYNECHOCYSTIS, NATIVE ENZYME
COMPND    APOCAROTENOID-CLEAVING OXYGENASE
 ObjectMolecule: Read secondary structure assignments.
 ObjectMolecule: Read crystal symmetry information.
 Symmetry: Found 4 symmetry operators.
 CmdLoad: "2BIW.pdb2" loaded as"2BIW.pdb2".
```

Note: XXXX substituted for 2BIW within the saved PDB text because we opted to select only a portion of the original PDB data when we chose to use a biological subunit rather than the complete entry. The XXXX reflects that this is a partial, or altered PDB file.

Note: why not use the **File> Open** menu sequence? Good question… You can actually try that option and it might work on your current system. However you will likely find that when you get to the *Open* entry of the files you want to open are shown in gray and therefore cannot be opened. The easy fix is to rename the file from *.pdb1 or *.pdb2 to simply *.pdb before you try to open it.



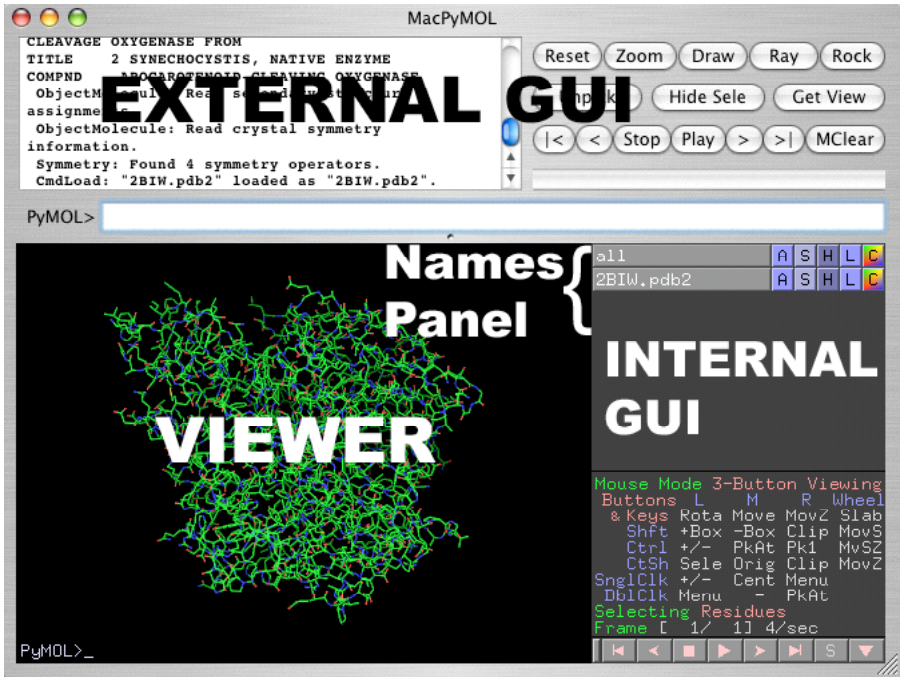
The load line-command option circumvents all file naming convention issues.

3 *PyMol - Exercise C*: Understanding the PyMol interface

READ

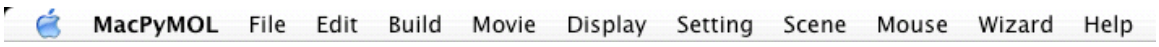
This exercise continues on the previous exercise where 2BIW.pdb2 was loaded within the PyMol software.

Your screen should be similar to this image without the extra markings.



The Viewer and Internal GUI are the parts we will use most.

The default size of the image in the viewer is 640 x 480 pixels.



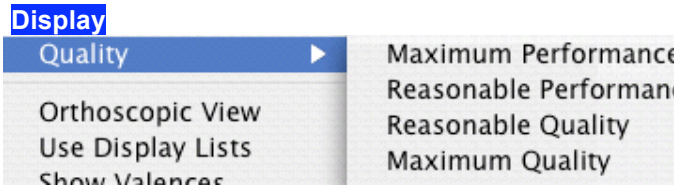
Note:The menu bar might be attached to the external GUI in other systems.

By default PyMol will display the molecule(s) contained within the PDB file as a wireframe. This cyanobacterium molecule is a carotenoid oxygenase and contains a carotenoid ligand.

3.1 PyMol settings to work on a very slow (laptop) computer

INFO

The Display > Quality menu cascade allows you to adapt to the speed of you machine CPU depending on the quality of the image displayed in the Viewer. This option MAY affect the result of ray-traced images Ray-traced images are explained below.)



The DMC computers are recent and powerful. However, if you are using PyMol on a slow computer or very slow laptop, choose the “Maximum Performance” to work faster.

3.2 Mouse control of the 3D representation

The 3D molecule is represented within a virtual 3D world. The flat surface of the screen represents the X and Y axes while the Z, depth axis is perpendicular to the screen.

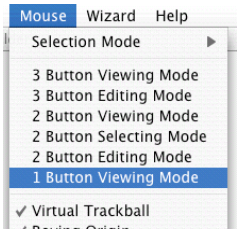
PyMol is optimized for a 3-button mouse but most basic functions can still be achieved by a one-button mouse, in particular the rotations around X, Y, and Z.

Rotation around the X or Y axis:	(left) click and drag.
Rotation around the Z axis:	(left) click on the top left or right corner.
Translate (move sideways) X or Y:	click middle button and drag.
Zoom (move along Z axis):	click right button and drag up or down.

3.3 Changing the default mouse settings

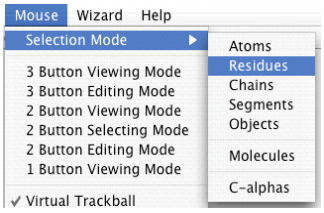
INFO

By default **PyMol assumes that you have a 3-button mouse**. If you have a 2- or one-button mouse you can change the setting accordingly with the “Mouse” menu in the top menu bar.
Note the updating of the “Mouse Mode” button mapping at the bottom right within the “Internal GUI if you change the mouse setting.



Note: the **Selection Mode>** submenus define what is selected when an atom is clicked on.

The selection default is Residues.



3.4 Show menu (S): Changing the representation style of the molecule

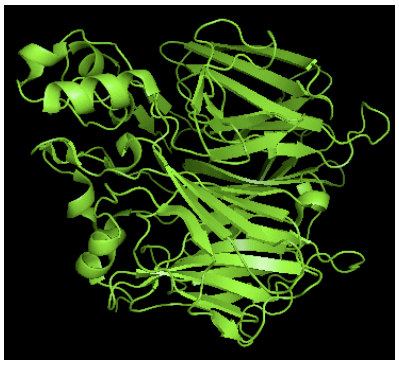
READ

PyMol can open more than one molecule at a time, or separate complex PDB files into individual components. Each opened or loaded molecule is given a name within the “Names Panel” (see picture above). The first name is always “all.” Clicking on the name itself will undisplay the corresponding molecule(s) (temporarily invisible).

The ASHLC menu (A S H L C) is abbreviated for **A**ction, **S**how, **H**ide **L**ablel and **C**olor. Some menu items have submenu components. Selections made under the "all" line will affect all the opened molecules.

Rule: Once a selection is shown (S) it must be selectively hidden (H) as it is not removed when another selection (S) is made. Selections are therefore additive, which allows for the creation of complex images with mixed graphical representations.

3.5 Cartoon



✔ **TASK**

Let's first make a cartoon representation of this protein: within the 2BIW line:

- ✓ **click S** and
- ✓ **select Cartoon**.

The molecule is now shown as both cartoon and wireframe.

Remove the wireframe by **clicking H and lines**.

(Note that within the S submenu list, the "**as**" menu contains a lot of redundancies.)

Options: most options can be set within the "Setting" menu within the top menu bar.

For example, it is possible to change the way all alpha helices are rendered.

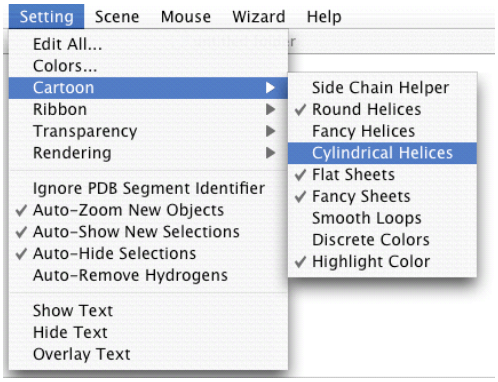
✔ **TASK**

Follow the menu cascade:

Setting > Cartoon > Cylindrical Helices

Select this option again to remove its effect and do the following:

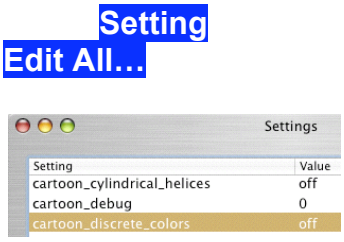
Setting > Cartoon > Fancy Helices

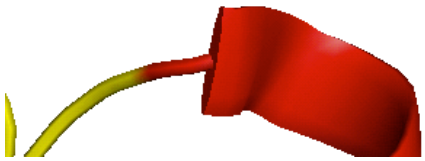


Testing other cartoon settings: Engaging the option **Smooth Loops** will simplify the drawing. Removing the option **Highlight Color** will make the edges of strands and inside helices surfaces a gray color (default).

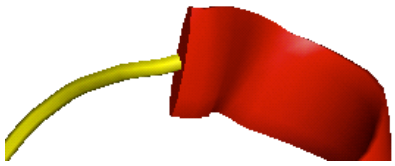
INFO Cartoon Options:

Turning the variable cartoon_discrete_colors on makes the helix color end abruptly at the ends of the helix. The default value is off. The change can be done manually with the menu cascade **Setting > Edit All…** or can be given as a typed command: **set cartoon_discrete_colors = on** (the blank space on either side of the = sign is optional).





set cartoon_discrete_colors = off

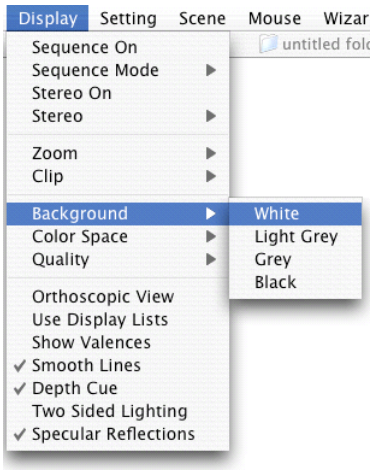


set cartoon_discrete_colors = on

3.6 Background color

Black backgrounds look very nice on the screen but do not print well on paper and do not photocopy well. Changing the background to white is usually very useful:

The "Display" menu within the top menu bar contains options for most options pertinent to displaying the image witin the PyMol viewer.



TASK

To change the background color to white follow this menu cascade:

Display > Background > White

Note that there is "fog" within the back of the molecule, which can be toggled on and off with the **Depth Cue** menu item within this same menu list.

Changing the color of the ribbon is easy with the following cascade menu within the PyMol “Names Panel” of the “Internal GUI” under the C menu as shown in the following menu cascade:

✔ **TASK**

2BIW.pdb2 > C > oranges > orange

You may also choose another option which is to color by secondary structure by following this menu cascade instead:

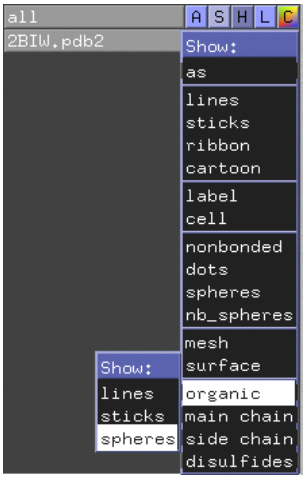
2BIW.pdb2 > C > by ss > Helix Sheet Loop

(choose one of the proposed color options displayed e.g. red-yellow-green.

3.7 Displaying (adding) ligand

When we opted to show the molecule as a cartoon above, one thing happened: the protein was shown as the familiar cartoon representation, but any ligand such as co-enzymes, substrates or inhibitors (which is the true for this file) it simply does not appear as it is not part of the cartoon representation of the protein. Here we will “rescue” the ligand!

This menu cascade is also within the “ASHLC” menus of the PyMol “Internal GUI” “Names Panel.” Since ligands are usually small, organic molecules, the following cascade within the **Show** menu for line 2BIW will show the ligand. Perform the following cascade:



✔ **TASK**

2BIW.pdb2 > S > organic > spheres

This cascade will select the carotenoid present within the PDB file.

Note that it is the same color as other parts of the protein, as it is part of the name 2BIW.pdb2 line. It will be either orange or the color for loops in the C/ss/Helix-Sheet-Loop color scheme chosen in the step above.

3.8 Surface representation

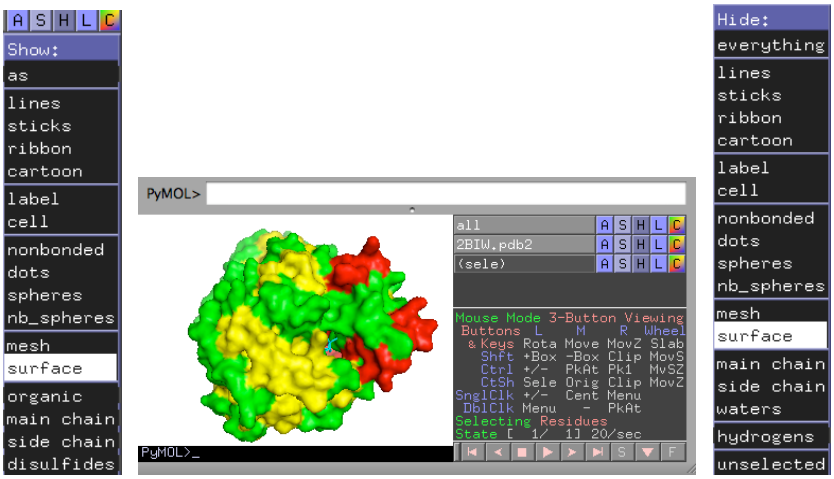
Surface representation used to be extremely computationally intensive. However, PyMol offers very fast and beautifully rendered surfaces.

✔ **TASK**

Using the show (S) menu, display the surface of the protein, then hide it with the H menu:

2BIW.pdb2 > S > surface

2BIW.pdb2 > H > surface



3.9 Mouse selection

Now that we have made the ligand visible, it becomes easier to select it with the mouse to make further changes.

✔ **TASK**

Click on one of the **spheres** of the **carotenoïd ligand**. This simple click makes various things happen:

- pink, square dots appear onto all the spheres of the ligand, indicating that it has been selected.
- A new name line appears within the “Names Panel” GUI called “(sele)” and is now dedicated to this subset of atoms. Note that the content of (sele) changes as other atoms are clicked
- The name of the atom that was clicked appears within the top text window of the “external GUI.” For example:

```
You clicked /2BIW.pdb2//B/TYR`322/OH
Selector: selection "sele" defined with 12 atoms.
```

This could be read as “you clicked atom OH which is on the 322nd atom in the file, and belongs to Tyrosine 322 of chain B in the object created when opening file 2BIW.pdb2. The complete selection contains 12 atoms (which make up the complete Tyrosine without the hydrogens, since these are usually not present in PDB files.)

Now that the ligand atoms are segregated within the name of (sele) we can change its color if we want by the following cascade within the Names Panel:

✔ **TASK**

(sele) > C > by element > CHNOS….

(selecting the first CHNOS… after HNOS… in the list would display the ligand as green with one red oxygen).

3.10 Saving an image

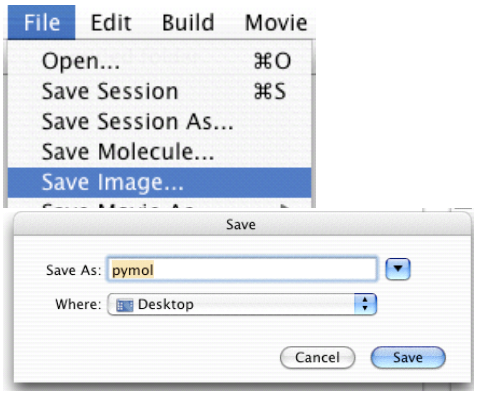
If you still see the selection dots over the ligand from the previous section simply click anywhere on the white background to unselect. Alternatively click on the "Hide-Sele" button at the top right hand side of the "external GUI."

TASK

Rotate the molecule to find a perspective that you deem instructive of the conformation of the protein and it's bound ligand.

Follow this menu cascade to save the image currently within the Viewer:

- **File > Save Image…**



Then replace the default word "pymol" to give a name to the file you want to save, e.g. image1

The image will be saved as a PNG image on the desktop.

INFO - Screen Capture:

If for any reason you cannot save the current image of your PyMol session, the following info is useful to capture the screen, or a portion of the screen:

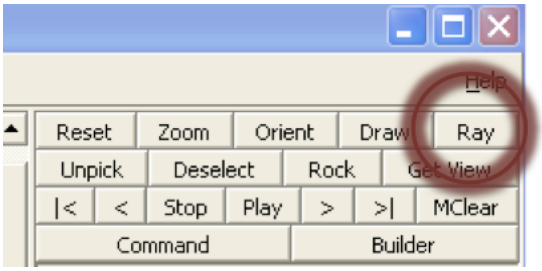
Macintosh		*Windows*	
Full screen:	⌘ + Shift + 4	Full screen:	Print Screen key
Screen selection:	⌘ + Shift + 3	Screen selection:	Shareware

3.11 Ray Tracing images

The previous image is rather crude in terms of graphics and resolution. PyMol offers an internal "ray tracer" to create stunning rendered images with a high visual quality much more pleasant to the eye and ideal for publication.

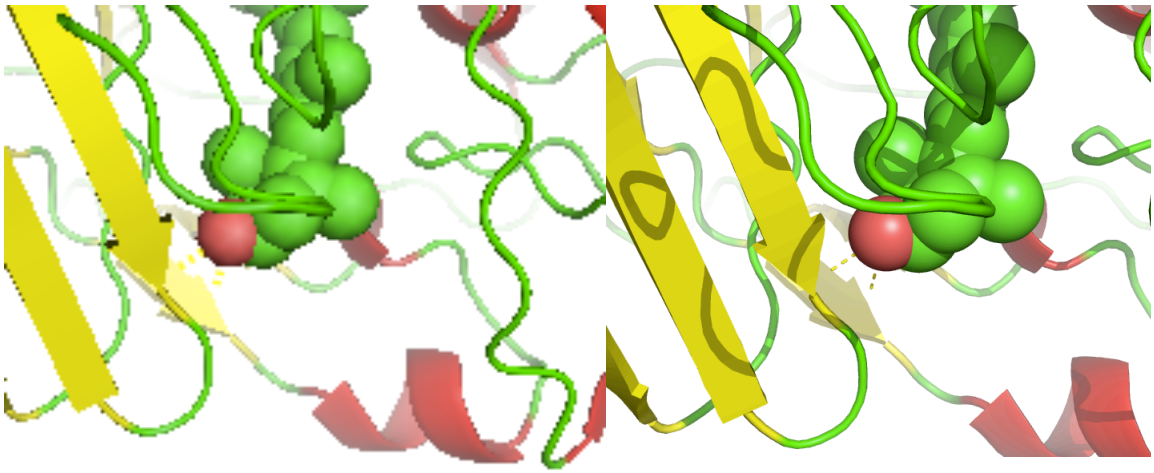
TASK

To create a standard ray-traced image of the current Viewer scene, **click the "Ray" button** at the top right of the "external GUI."



The rendering will take a few seconds to a few minutes depending on the complexity of the PDB file and the chosen display, and will also depend on the speed of the computer CPU. Once rendered, the image appears within the Viewer.

To save the file, use the save cascade as above: **File > Save Image…**



Zoomed side-by-side comparison between the pymol image and the ray-traced image: note the jagginess of the original image and the smooth appearance of the ray-traced image, with shadows as a bonus.

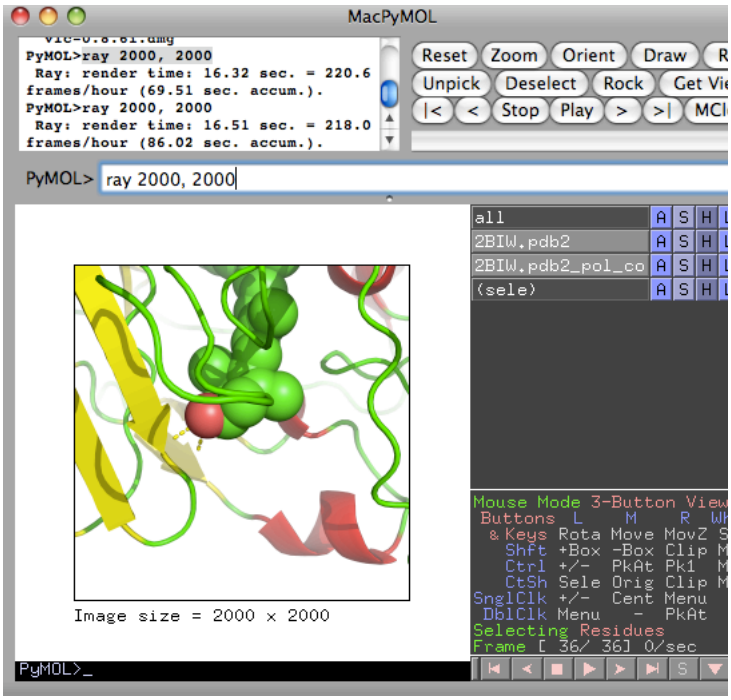
This is useful to create preview images for slide presentations, but is still one step short of the quality needed for high resolution publication, as the image created by the default setting is the same size as that of the current Viewer (default size is 640 x 480 pixels when PyMol is first opened.) The default file format is the new PNG standard. All we need to do at this point is change the default setting of the ray-traced file size.

✔ **TASK**

Within the PyMOL> line command type the following command to change the dimensions of the final ray-traced image:

ray 2000, 2000

(2000 is an example number. Note the comma between the two numbers. The higher the numbers the longer it will take to compute the image). PyMol will display the size of the calculated image within the Viewer under the image here 2000 x 2000



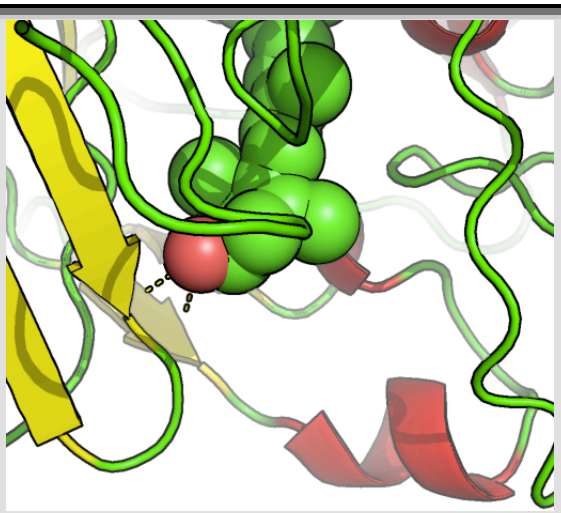
Note: **`ray 2000`** (typed within the line-command input) is also a valid command. In this case PyMol will evaluate the missing value and adjust it to minimize the file size.

✔ **INFO** - Ray tracing options:

There are 50 editable settings listed in the menu **Setting > Edit All…** for ray tracing! The following 2 are of special interest:

ray_shadows is "on" and can be edited within the settings window or the line command: **set ray_shadows, on** or **set ray_shadows, off**

ray_trace_mode has a default of 0 and can also adopt values of 1 and 2 to create contour-enhanced images or old-fashion black and white contours in the Jane Richardson style (that used to be hand-drawn!)



set ray_trace_mode, 1

set ray_trace_mode2

To render type **ray** or **click ray** button

Return to ray trace **defaults**: **set ray_trace_mode, 0**

3.12 Where is the HELP command?

✔ **READ**

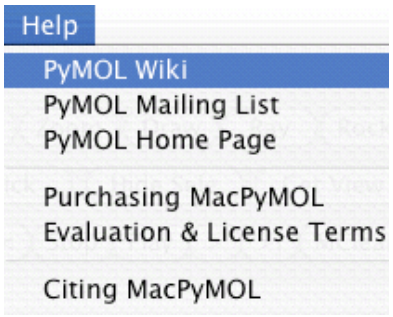
3.12.1 Web help

Some on-line web content can be called from the Help menu in PyMol. The default web browser is opened and content is displayed.

PyMol Wiki: http://pymolwiki.org/index.php/Main_Page
with links to other PyMol Wikipedia pages.

PyMol Mailing List opens the mailing list subscribe page, and offers links to archives

PyMol Home Page opens http://pymol.sourceforge.net/



3.12.2 Documentation

Older PyMol User's Manual and Pymol Reference Manuals are available online as HTML or PDF: http://pymol.sourceforge.net/html/

Newer documentation can be accessed for authenticated users (any connection from UW campus) at: http://delsci.info/dsc/dokuwiki/doku.php

3.12.3 Internal help

PyMol also offers an internal summary of all the command derived from the manual. These are called from the line command `help xxx`, where xxx is the name of the line-command, e.g. `help align` or `help color`.

The information displayed is essentially that of the reference manual and is shown both within the text area of the external GUI and within the graphical viewer. **Press the Esc. Key to go back to the graphical view.**

Note: PyMol is written with the language Python, and some specifics about this is given at the end of the help data. Unless noted, you do not have to remember these commands!

---

4 *PyMol - Exercise D*: Action preset menus

This is mostly a self-paced exploration of one of the menus that is sure to change over time as PyMol evolves.

Preliminary If you are not continuing this exercise from the previous exercise do the following tasks:
√ - load the structure 2BIW.pdb2 as in Exercise B;
√ - then click S> Cartoon to be in a similar sate as in the previous exercise.

4.1 Preset menus: automated complex imaging

The preset menu is part of the Action set of the ASHLC menus controlling the aspect of molecules from the Names Panel.

✔ **TASK**

Follow this menu cascade sequence to return to the default view, as when you just opened the molecule. No rotation will occurs:

2BIW.pdb2 > A > preset > default

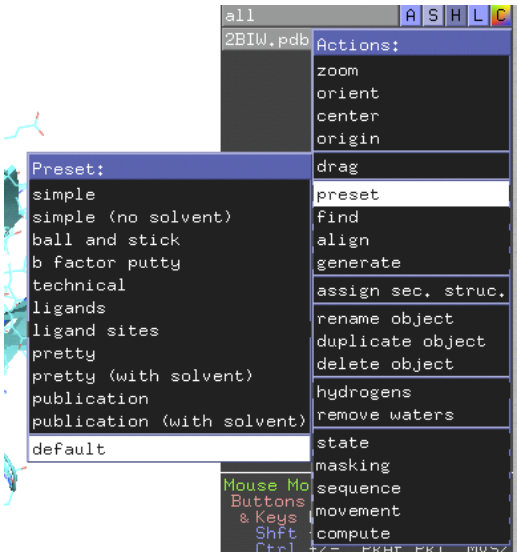
This command has a similar effect but is not the same as the following cascade:
“hide everything and show lines:”

2BIW.pdb2 > H > everything

and

2BIW.pdb2 > S > lines

Note: the "preset" options will set some variables that are specific to these views and may change further drawings. To remove the effect of these presets affecting an object representation, use the **A>preset>default** menu cascade reset parameters.

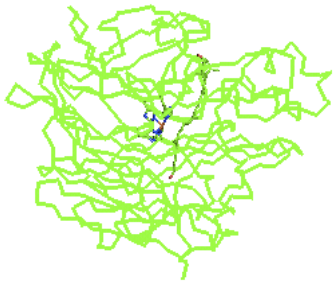


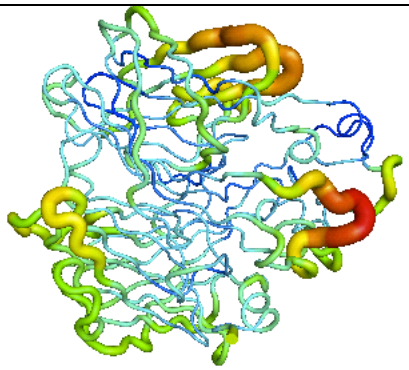
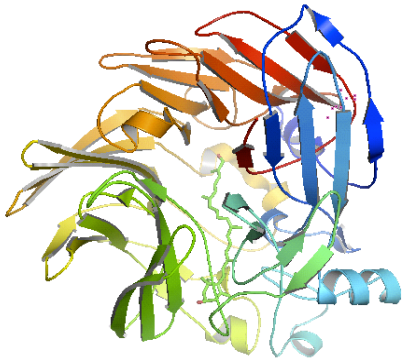
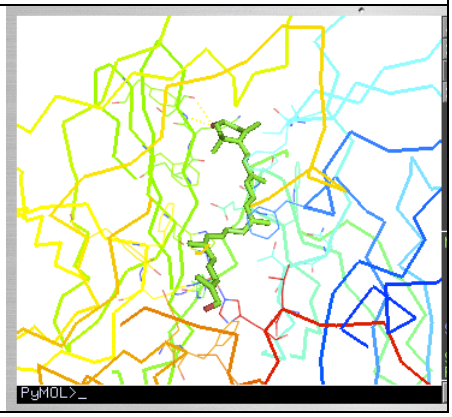
Note: to get back to the original opening view simply type **reset** at the PyMOL> line command.

4.2 Preset Options: Exploring more

✔ **TASK- Explore the other menus** of this series.

The cascade menu **2BIW.pdb2 > A > preset** is assumed in the following commands, just continue with the suggested command. E.g. for the first one the complete command would be **2BIW.pdb2 > A > preset > simple**

simple The tracing can then be made thicker by unselecting the smooth option with the following menu cascade: **Setting > Ribbon > Smooth** Note: a set of 3 histidines is also shown.	
ball and stick	This is not very useful for a large protein such as this.

b factor putty The segments with the highest temperature factor are shown as thicker cylinders. Regions of better resolution have thinner diameter and are usually found at the core of the protein. Mostly loops in the outside of the protein wobble: the core portions of the proteins usually appear more stable than the external loops. This is mostly useful for crystallographers but is a cool representation.	
technical	Color domains in separate rainbow colors and shows backbone and side chains. Note that a subset name appears in the Names Panel (2BIW.pdb2_pol_co) that control the dashed-line hydrogen bonds
pretty and *publication* create similar images of a rainbow color cartoon with a stick ligand. Pretty creates the default cartoon setting, while publication creates an image very similar to an image created by Molscript*. (* Per J. Kraulis 1991: MOLSCRIPT: A Program to Produce Both Detailed and Schematic Plots of Protein Structures. *Journal of Applied Crystallography*. 24: 946-950. http://www.avatar.se/molscript/)	
ligands This option will zoom in on the ligand site and show the protein as backbone except in the near vicinity of the ligand where side chains are shown. The ligand is depicted as a thicker cylinder. Note: to zoom out, simply click on the A in the ASHLC menu again.	

ligand sites

There are a few options available in this submenu, all pertinent to looking closely at the ligand in it's binding pocket.

You can explore a few of them on your own, once you are done then select the following option: **preset > ligand sites > solid surface**

You should obtain a centered, zoomed view of the ligand shown as a stick model within a partial molecular surface pocket. The colors are the scheme of previously chosen colors, for example if you tried the "technical" preset earlier the coloring would likely be like a rainbow.

✔ TASK

This quick change will make a much nicer image:

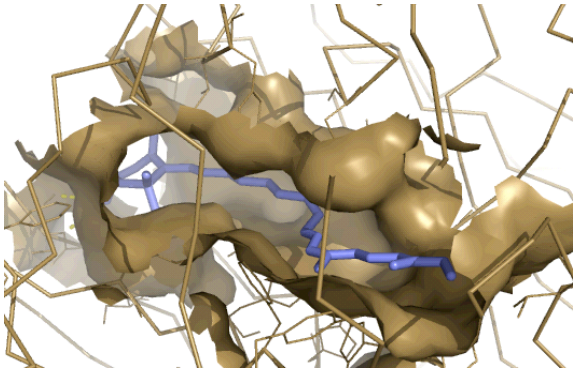
2BIW.pdb2 > C > yellows > sand

Now with the mouse click carefully anywhere on the ligand stick to select it. As before you will have a (sele) name within the Names Panel. You can now change the color with the following menu cascade: **sele > C > blues > slate**

Of course you can pick your own colors. Make sure that there is sufficient contrast between the color of the surface and the color of the ligand.

If you have not yet done so, **rotate the molecule** to select a nice viewing angle.

If you want to add a more stunning effect **click on the "ray"** button as we did before to complete your publication quality picture.



Note: If you are preparing a figure for a black and white print publication, it might be advantageous to use the various gray scales, black, and white within the "grays" option.

5 *PyMol - Exercise E*: Sequence Viewer

Preliminary: We are still working with the 2BIW.pdb2 file loaded above. Review exercise B if you need to reload the structure.
This exercise assumes you have just completed creating the above view with the preset menu cascades with the suggested colorings :

√ - 2BIW.pdb2 > A > preset > ligand sites > solid surface
√ - 2BIW.pdb2 > C > yellows > sand
√ - Click on the ligand to obtain a selection (sele) that contains it
√ - (sele) > C > blues > slate

5.1 Sequence viewer

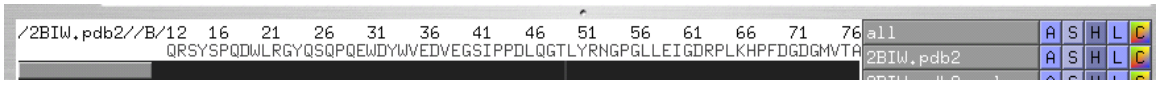
The molecule sequence can be shown at the top of the graphical area.

✔ **TASK**

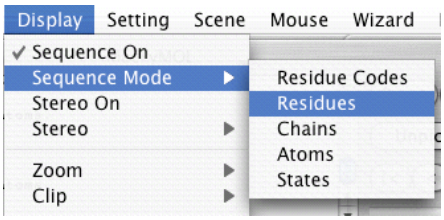
To engage sequence viewing follow the top menu cascade:

Display > Sequence on

The sequence appears just below the PyMOL> line command at the top of the Viewer. The slide cursor underneath can be used to move the sequence viewed further.


/2BIW.pdb2//B/12 16 21 26 31 36 41 46 51 56 61 66 71 76
QRSYSPQDWLRGYQSQPQEWDYWVEDVEGSIPPDLQGTLYRNGPGLLEIGDRPLKHPFDGDGMVTA
all
2BIW.pdb2
A S H L C

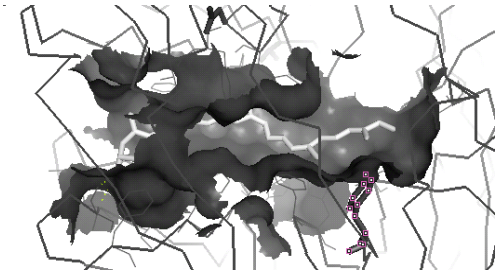
By default the one-letter code is displayed. Since we are looking at a protein, changing the display to the three-letter code will be useful within the next step .



✔ **TASK**

Display > Sequence Mode > Residues

With the mouse **rotate the molecule** to a view similar to that shown at right.



With the mouse, **click on** the **tyrosine** residue under the right hand side, which contribute to the pocket surface Change it's aspect to stick with the following menu cascade: **(sele) > S > sticks**

Note: When you clicked, the following text appeared within the text window:

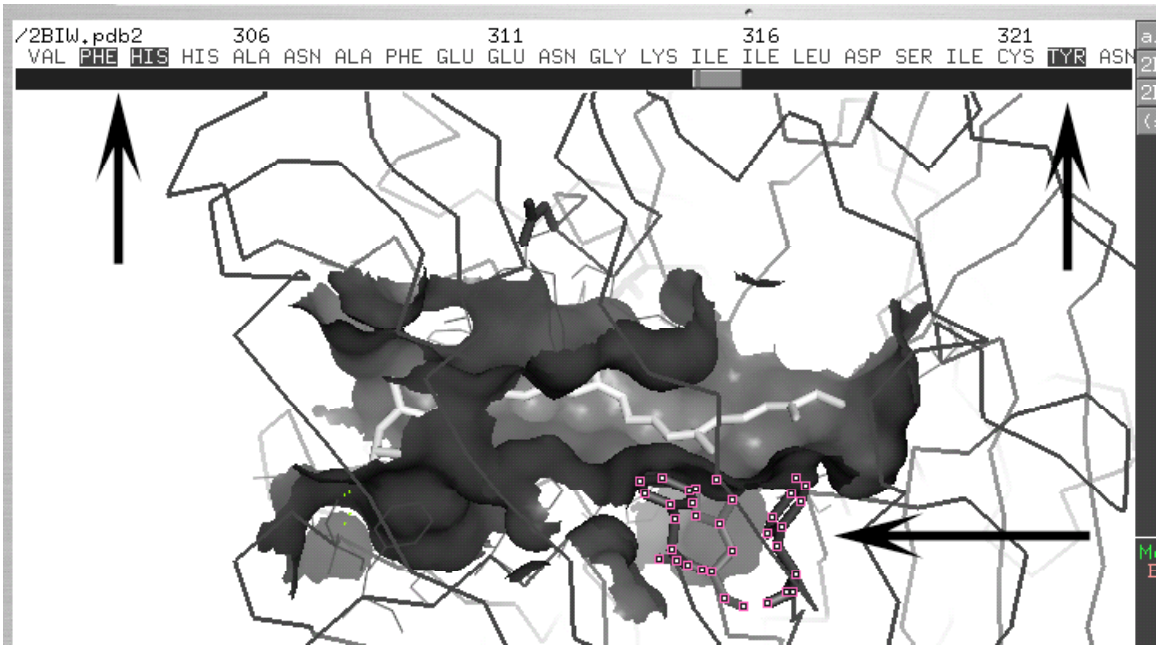
"You clicked /2BIW.pdb2//B/TYR`322/CG"

Therefore we know that Tyrosine 322 is the residue we chose (see below for explanation on the nomenclature.)

Now **slide the sequence cursor to the right** to move the sequence displayed until you find the region of the selected TYR. If you have the one-letter code engaged, it appears under the number 321. However we know it is 322. If you have engaged the three-letter code as instructed above TYR 322 is shown highlighted within the sequence line.

Display the sequence line to see residues PHE 303 and HIS 304. With the mouse click on residue 303 and residue 304 within the sequence line. Note that they are selected within the graphical window. The arrows within the following image show where you should look. As before, transform those side chains to a thicker stick with the menu cascade:

(sele) > S > sticks



Quiz question: We just selected amino acids TYR 322, PHE 303, and HIS 304. Can you describe with one word one important quality of this binding pocket?

*Answer: This binding pocket has the following quality:*_____

INFO

The sequence viewer can also be engaged by clicking on the “S” at the bottom right of PyMol where other reminders are shown.

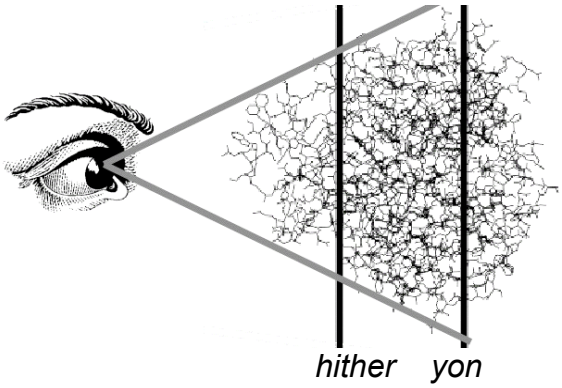
---

6 *PyMol - Exercise F*: Clipping planes & distance measurements

6.1 Clipping planes

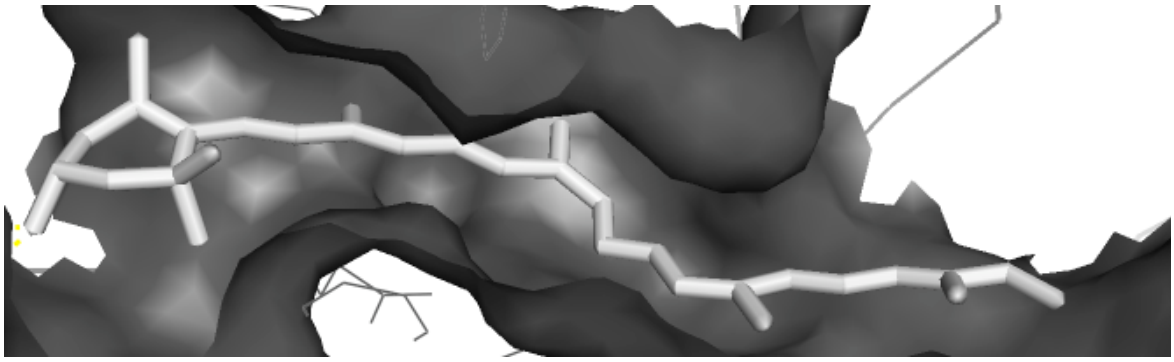
Clipping planes are imaginary planes in the front and back of the molecule. Parts of the molecule that are outside the planes are “clipped” and therefore invisible. This is very useful for complex or large structures.

This image represents the molecule seen side-ways “inside” the computer monitor.
The 2 black lines represent the *yon* (far away) and *hither* (close) clipping planes. These are parallel to the flat screen of the computer monitor display. The gray lines converge toward the user’s eye, who is looking at the molecule on the computer screen.



TASK

The DMC computers are equipped with 3-button mice. To move clipping planes **press shift** and the **right mouse** button **simultaneously** while dragging up and down. The same result can be obtained by using the **middle button scroll wheel**.
As an exercise, try to remove some of the molecular surface covering the ligand to create a picture similar to this:



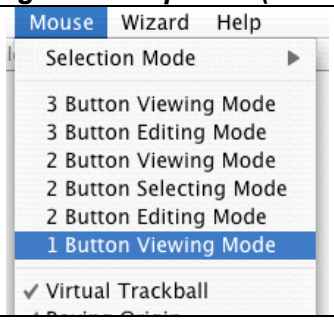
Note: we have seen previously that the top menu “Mouse” contains all the possible options, with a reminder displayed at the bottom right of the “Internal GUI” The method to adjust the clipping plane will depend on the number of buttons on your mouse. Use the “Mouse” menu to adapt your display to your mouse.

Depending on the mouse-viewing option (see exercise above about choosing mouse viewing) it may be necessary to use different mouse + keyboard strokes.

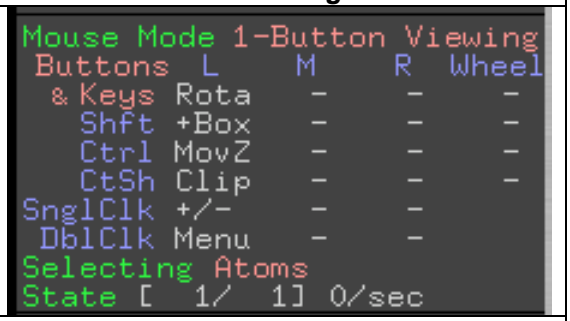
When the mouse option is changed, the bottom right panel of the graphical GUI changes)

INFO

Changing mouse options (review)



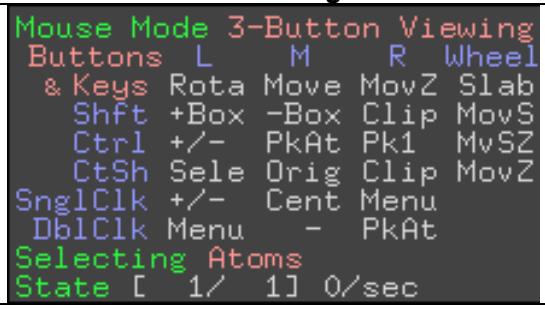
1-button mouse viewing


Mouse Mode 1-Button Viewing
Buttons L M R Wheel
& Keys Rota - - -
Shft +Box - - -
Ctrl MovZ - - -
CtSh Clip - - -
SnglClk +/- - -
DblClk Menu - -
Selecting Atoms
State [1/ 1] 0/sec

2-button mouse viewing

Mouse Mode 2-Button Viewing
Buttons L M R Wheel
& Keys Rota - MovZ -
Shft Pk1 - Clip -
Ctrl Move - PkAt -
CtSh Sele - Cent -
SnglClk PkAt - Menu
DblClk Menu - Cent
Selecting Atoms
State [1/ 1] 0/sec

3-button mouse viewing


Mouse Mode 3-Button Viewing
Buttons L M R Wheel
& Keys Rota Move MovZ Slab
Shft +Box -Box Clip MovS
Ctrl +/- PkAt Pk1 MvSZ
CtSh Sele Orig Clip MovZ
SnglClk +/- Cent Menu
DblClk Menu - PkAt
Selecting Atoms
State [1/ 1] 0/sec

Regardless of the number of buttons on your mouse, simply look at the bottom right to see the corresponding mouse + keyboard action for the following 2 items: **MovZ** and **Clip**.

MovZ will move the object closer or further from your point of view.

Clip will reduce the size of the box into which the object is represented and increase the contrast with depth-cueing, making parts of the molecule that are further back much darker.

Playing with these 2 items, it is possible to increase the feeling of depth and 3D feeling of any represented object and particularly surfaces with deep pockets.

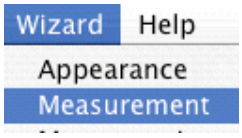
You need to make sure however that the the “depth-cue” option is engaged within the menu “**Display**.”

6.2 Measuring distances with the Measurement Wizard.

Distances are measured between two atoms and are expressed in the same unit as the XYZ coordinates within the PDB file: Angstroms (1Å = 10^{-10} m).

As an example we shall measure the distance between two atoms within the carotenoid ligand.

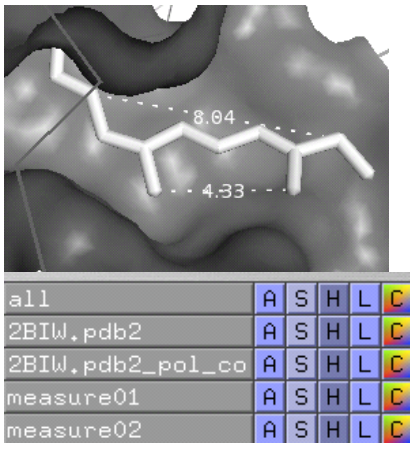
Within the top menu select
Wizard > Measurement
(Note: in older PyMol versions Measurement was called Distance.)
This will create a prompt within the Viewer:
“ **Please click on the first atom…**”



Within the “Internal GUI” a “Measurement” table also appears. It can also be used to remove measurement objects after they are no longer needed.

Click on the **first** atom **on the ligand**
Click on the **second** atom **on the ligand**

(you can select the same atoms as in the examples within the image at right, or select your choice of atoms)

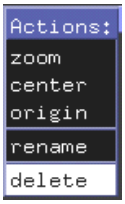


The default color of the measurement object is yellow. This can be easily changed with the familiar ASHLC menu for each measurement, as a new name is entered within the “Names Panel” for each distance, e.g. “measure01.”
Change the color to white with the following menu

cascade: **measure01 > C > grays > white**

Quiz exercise: you can also measure the distance between the OH at the tip of TYR 322 and the nearest ligand atom (C30).
Answer: _____

When you are done using the "Measurement" panel on the bottom right **click Done**. If you no longer need to display the distance object, **click Delete All Measurements**.



Alternatively you can use the corresponding "A" menu and select the delete option.

✔ **INFO** - Distances are labels

The display of a distance measurement is a label. To alter the number of decimal digits reported change the label setting label_digits from default 1 to the desired value with either the **Setting > Edit All…** menu cascade or the line command: **set label_digits, 2**

7 PyMol - Exercise G: Labels

7.1 Labels

✔ **TASK: Click on TYR 322** to have it within the **(sele)** name.

A label containing the residue type and sequence number (e.g. TYR 322) can be added to a selected residue with the menu cascade (sele) > L > residues

By default, labels are created the same color as the atom.

7.2 Label color

"How can I change only the label color without changing the display of the atom or molecule? "

You can change the label color to e.g. yellow with the following line command:

set label_color, yellow, sele

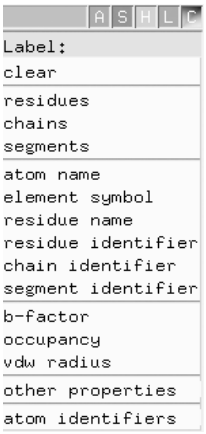
- Yellow can be changed for other colors (The **C** menu can be a source of inspiration for colors and color names.)
- sele represents the current selection. You can alter the command with the name of the object you are working on e.g. 2BIW.pdb2
- note the use of the comma (,) within the line command

For publications or slide making, labels could be added with e.g. Adobe (PhotoShop, Illustrator) or Microsoft (PowerPoint) graphic editing software.

✔ **TASK**

Explore the L menu, knowing that "clear" will remove the mess that may occur!

(on this image colors were inverted for easier reading.)



7.3 General label Settings

General default settings can also be altered generally:

✔ **TASK**

Open the Setting > Edit All… top menu and change settings as illustrated

Default label values

Setting	Value
isomesh_auto_state	off
label_angle_digits	-1
label_color	default
label_digits	1
label_dihedral_digits	-1
label_distance_digits	-1
label_font_id	5
label_outline_color	default
label_position	[0.00000, 0.00000, 1.750
label_shadow_mode	0
label_size	14.00000
legacy_mouse_zoom	off

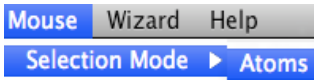
Label values changed

Setting	Value
isomesh_auto_state	off
label_angle_digits	-1
label_color	yellow
label_digits	1
label_dihedral_digits	-1
label_distance_digits	-1
label_font_id	5
label_outline_color	default
label_position	[0.00000, 1.50000, 1.75000
label_shadow_mode	5
label_size	32.00000
legacy_mouse_zoom	off

7.4 Labeling one atom

Text label can also be added within PyMol, although as suggested above, adding label within a graphical software might be more appropriate in some cases.

✔ **TASK**
Change the **mouse selection to Atoms**



Click on one atom within the carotenoïd

Will show pink square

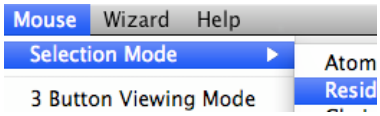
Within the text entry box type the following command:

```
label sele, "Ligand"
```

Note: the word in quotes, here "ligand" can be changed to any other word, such as "my molecule" or "carotenoïd" etc.

To clear the label, simply type: **Label sele**

✔ **TASK** Switch the **selection** mode back to **residues**



7.5 Greek alphabet

Letters from the Greek alphabet can be added to text-entered labels. The commands call on special fonts called Unicode UTF8 fonts. The Greek font is #316, the alpha letter is number 261 and omega is 277 (268 and 269 are not used.)

While alpha and beta might be most useful to label α-helices and β-sheets, the rest of the alphabet might be useful to label specialized items.

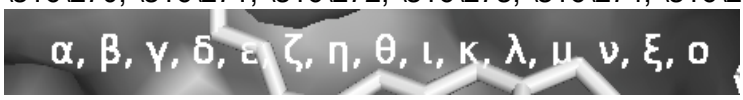
✔ **OPTIONAL**
Label the atom with alpha and beta Greek letters and some text:
Type the following commands within the text box:

label sele, "\316\261, \316\262: Greek Letters"
<press enter>
set label_size, 40

Or write part of the alphabet:

set label_size, 22

label sele, "\316\261, \316\262, \316\263, \316\264, \316\265, \316\266, \316\267, \316\270, \316\271, \316\272, \316\273, \316\274, \316\275, \316\276, \316\277"



7.6 More information

There are too many aspects to labeling. Exhaustive information can be found at:

http://www.pymolwiki.org/index.php/Label

---

8 *PyMol - Exercise H*: Saving a PyMol session

A session file is a binary file containing all the information and graphical displays currently within PyMol. It is a way to save the “current state”of the software with all that it contains. Later, the file can be opened and everything is restored.

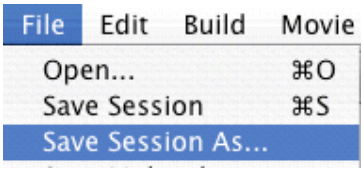
8.1 Saving the session file

✔ **TASK**

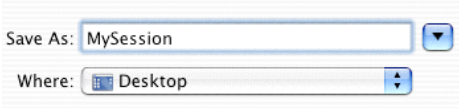
From the top menu follow the menu cascade:

File > Save Session As…

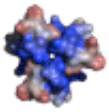
8.2



In the next window enter a name: **MySession** and save the resulting file on the **Desktop** to easily find it again.



The susscessful writing of the file will be reported within the text window of the “External GUI” and a file called Mysession.pse on the desktop (.pse is added automatically).



MySession.pse

Now quit PyMol: **File > Quit**

8.3 Restoring the session file

While it is possible to simply double click on the MySession.pse icon, this could create problems if there are multiple copies of PyMol within your computer and

even more so if they are various versions of the software. It is therefore best to first open the PyMol software version you want to utilize.

✔ **TASK**
For this exercise: **double click** on the **Applications > Classes > MacPyMol** software to open it.

Within the PyMol top menu follow the menu cascade: **File > Open…..**
and then **select Mysession.pse** from the Desktop.

All the PyMol names and selected items are restored as if you had just made them, even if days have passed since you saved the file. How convenient!

Note: the file has a binary format. There is no information within the file that is useful for any other purpose. The file for this exercise should likely be slightly less than 1Mb in size.

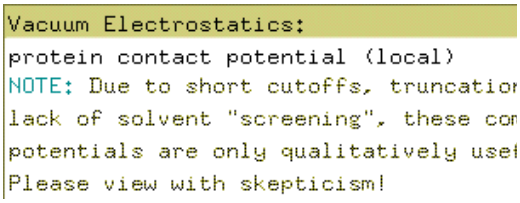
---

9 *PyMol - Exercise I*: Electrostatic potential

The most accurate potential maps can be calculated by external software (Grasp, Delphi, APBS, MEAD) and displayed in PyMol.
A tutorial example for APBS is available online at

`http://www-bio3d-igbmc.u-strasbg.fr/doclib/apbs/tutorial/index.html`

PyMol offers an approximate map nicknamed "*charge-smoothed*" surface representing approximate charge distribution on the protein surface. Assuming that you have opened PDB file 2BIW.pdb2, the potential surface is calculated and displayed with the following menu cascade on the Names Panel:

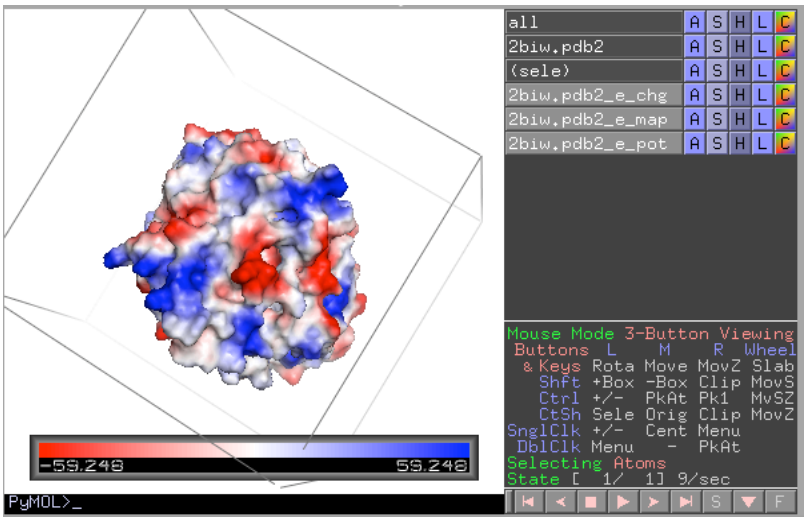

Vacuum Electrostatics:
protein contact potential (local)
NOTE: Due to short cutoffs, truncatio
lack of solvent "screening", these co
potentials are only qualitatively use
Please view with skepticism!

(Note: for reading clarity colors are inverted)

9.1 calculating and displaying a map:

✔ **TASK**

2BIW.pdb2 > A > generate > vacuum electrostatics > protein contact potential (local)



The process creates 3 new entries within the Names Panel: 2BIW.pdb2_e_chg, 2BIW.pdb2_e_map, and 2BIW.pdb2_e_pot (2BIW.pdb2 is subsequently abbreviated X below.)

X**_e_chg** is an object containing the surface, colored red/white/blue and is an approximate map.

X**_e_map** is usually not shown (**click on name to show**) and displays the volume boundaries as e.g. a big cube.

X**_e_pot** is the object representing the color ramp and value at the bottom of the display.

9.2 Adjusting color levels with the mouse:

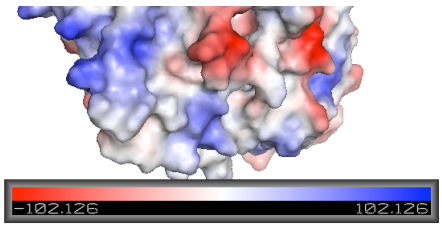
With protein 2BIW the default values for red and blue are -55.248 and +55.248 respectively.

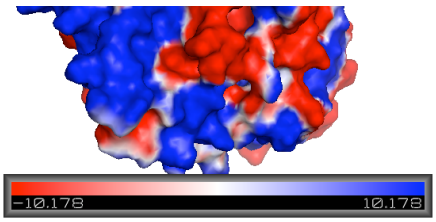
It is possible to adjust the color level with the middle button and the control key.

✔ **TASK**

√ **- Place** the **mouse** over the color scale
√ **- Hold the CTRL** key and **click** on the **middle button**.
√ **- Adjust** the color level by **sliding the middle button**
√ **-** Go first to a **range near +/- 100**
√ **-** Then to a **range near +/- 10**

Note: Do not go all the way to -0 +0 as it then becomes virtually impossible to slide to proper values after that.





9.3 adjusting the value range and color strength with line command

If two proteins are present, the process has to be applied to each individual protein, and the same _e_ objects are created for each one. The values within the X_e_pot color ramp may be different for each protein. Therefore it is useful to know how to change the values within. Smaller numbers will increase the blue and red strength and contrast within the blend of white surface, while larger numbers will dim the colors.

✔ **TASK**

To change the color range within the ramp:
(example): ramp_new 2BIW.pdb2_e_pot , 2BIW.pdb2_e_map, [-100,0,100]

9.4 Adjusting the display colors

The default colors are red/white/blue, hence the above command could also be rewritten to change ramp values and specify colors:

ramp_new 2BIW.pdb2_e_pot , 2BIW.pdb2_e_map, [-100,0,100] , [red, white, blue]
or
ramp_new 2BIW.pdb2_e_pot , 2BIW.pdb2_e_map, [-100,0,100] , [[1,0,0], [1,1,1] , [0,0,1]]

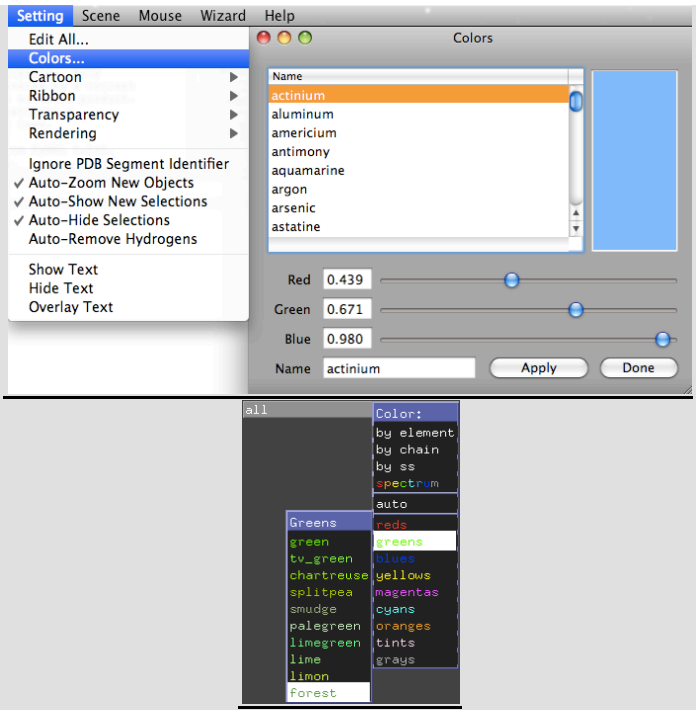
where [[1,0,0], [1,1,1] , [0,0,1]] represents the [R, G, B] (red/green/blue channels) values for each of the 3 displayed colors. To change the displayed color, simply change the definition of the colors. For example, the values **[[1,1,0], [1,1,1] , [0,1,1]]** would create a ramp as yellow/white/cyan.

INFO

An alphabetical list of all PyMol-defined color names can be found under the top menu "**Setting > Colors…**"

Within that window the colors can also be edited.

The **C** menu within the Names Panel offers a list of color names grouped by tint and can serve as a preview.



9.5 Default display:

Note that when the calculation first takes place, the surface is shown but the original PDB file is hidden. In the case of 2BIW it means that the carotenoïd becomes invisible. To restore it, simply click on button 2BIW.pdb2 within the Names Panel: this will restore the display of the protein and ligand as lines or sticks. Since the protein is under the surface it will remain invisible (but some odd side chains might stick out of the surfaces.) To make more complex images it may be useful to create a new object containing the ligand alone (see creating objects below.)

9.6 Deleting the calculated maps:

2BIW.pdb2_e_chg, 2BIW.pdb2_e_map, and 2BIW.pdb2_e_pot are PyMol objects that can be deleted with the A (action) button. Note: the menu will be different for the 3 objects within the A menu!

TASK

Delete the 3 objects pertinent to the electrostatic potential :

2BIW.pdb2_e_chg > A > delete	2BIW.pdb2_e_map > A > delete	2BIW.pdb2_e_pot > A > delete

10 *PyMol - Exercise J*: Creating new objects; automatic zooming.

10.1 Making a new object from selection

The current selection (sele) as well as other subsets are shown within parentheses and represent subsets of the current PDB file we are working on (e.g. 2BIW2.pdb2). Any selection can be copied into an independent object with the **"A" Actions: copy to object** menu cascade. This will create a new entry within the "Names Panel" without the parentheses that becomes independent of the original PDB file.

✔ **TASK**

For example, the ligand can be made into a separate entry:

√ - **Click** on the **ligand** (becomes the current (sele))
√ - **Click** on the **A** on the (**sele**) line and choose: **copy to object** (a new entry called obj01 appears within Names Panel, and an automatic zooming occurs)
√ - **Click** on the **S** on the (obj01) line to change the object appearance, e.g. as stick.

Note: If you make obj01 invisible by clicking on the obj01 icon, the ligand is still visible because it is also part of the 2BIW.pdb2 file!

Note: If the option "extract object" was used instead, the ligand would have been removed from the 2BIW.pdb2 object and would no longer be available under that name.

Therefore the 2 options both create a new object, one makes a copy of the original, and the other moves it.

10.2 Making a surface for the ligand itself

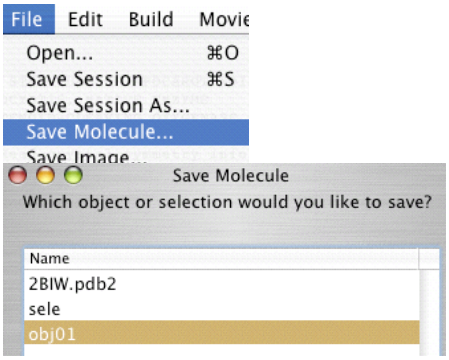
Question: Why can't I make a surface for the ligand itself?

Surfaces are reserved for ATOM records only. Typically ligands are stored as hetero-atom HETATM records (but authors of the PDB file may choose otherwise, hence always check within the file with a word processor.)

One way to circumvent this is to make the ligand into an independent object (see pervious paragraph), save it from PyMol into a text file, replace the ATOM word with HETATM and reopen the file with PyMol:

✔ TASK

Assuming you have created obj01 as described above, use the menu cascade
File > Save Molecule….



Choose **obj01** within the Save Molecule panel.

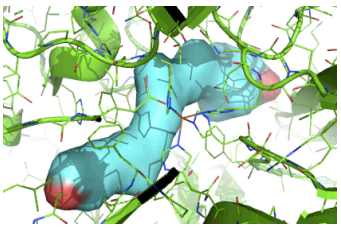
Choose a file **name** and save the file e.g. obj01.pdb. The file will be a PDB file with only the object 3D data and contains HETATM and CONECT records.

With a word processor open the PDB file and replace "HETATM" with "ATOM__" (ATOM *with 2 blank spaces* to respect the column positions!!!!!)

✔ TASK

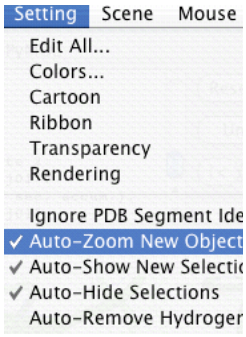
Delete the current obj01 with the menu cascade: Names Panel: **obj01 > A > delete object**

Open the PDB **file obj01.pdb** with PyMol (menu cascade **File> Open** or use the "**load**" line command)
A new obj01 now appears within the Names Panel, and the S > surface menu is now working for this object!


ray-traced example

a. turning off automatic zooming and clipping with new objects

When we created object obj01 from (sele) above, the default action of PyMol was to automatically zoom to the new object (in that case the ligand) and reduce the clipping planes. That can be annoying in some cases, but could always be reversed with the line command “reset” or with the menu **Display > Clip > None** or with the **Display > Zoom** menu options.



This option is turned off by un-checking the menu item: **Setting > Auto-Zoom New Objects**

11 *PyMol - Exercise K*: Side chain mutations

PDB files show the structure of a particular sequence and conformation. However sometimes it is useful to mutate a side chain to see what the effect might be.

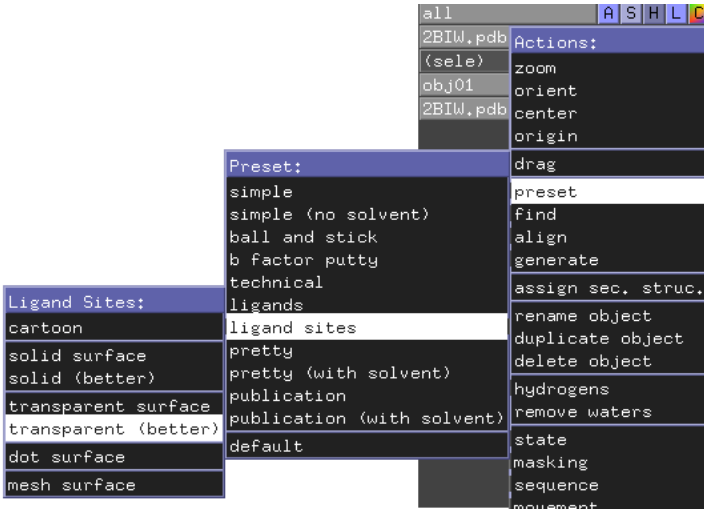
11.1 Preliminary: create a standard view to work with

✔ **TASK**

√ - Follow the menu cascades:

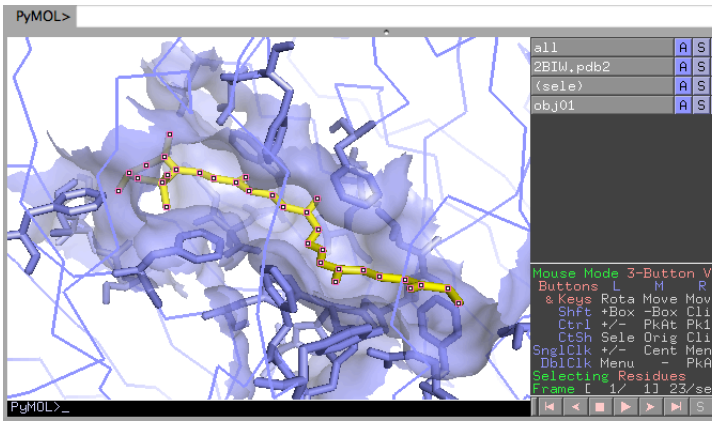
2BIW.pdb2 > A > preset >ligand stes > transparent

This will create a similar view of the ligand within the pocket with some amino acid sides chains shown as sticks.



The default colors are rainbow. To make the display clearer, change the colors with the following cascade menus:

√ **- 2BIW.pdb2 > C > blues > slade**
√ **- Click on** the **ligand**
√ **- (sele) > C > yellow**



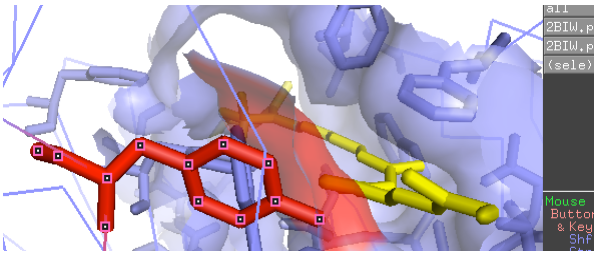
11.2 Select side chain to mutate

Since we already worked with Tyr 322 above, we shall use this as an example.

✔ **TASK**

√ **- Rotate** the **view** to **find Tyr 322**
√ **- Click** within the **blank area** to un-select previous (sele)
√ **- Click** on **Tyr 322** with the mouse to select it
√ **- Change it to red: (sele) > C > reds > red**

(note that the surface associated with Tyr 322 will also change color.)



11.3 Mutagenesis Wizard

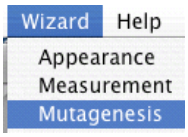
The menu cascade Wizard > Mutagenesis opens a new panel below the Names Panel and above the mouse control reminder. Directions will be prompted with text overlaid on the Viewer:

"Pick a residue" and "Select a rotamer, or pick a new residue…"

✔ **TASK**

Steps to mutate one amino acid side chain on a protein structure:

- Open from the menu **Wizard > Mutagenesis**



- When "Pick a residue" appears at top left, **Click on Tyr 322**

The text section will echo:

```
You clicked /2BIW.pdb2//B/TYR`322/CG
Selector: selection "sele" defined with 0 atoms.
You clicked /2BIW.pdb2//B/TYR`322/CG
Selector: selection "sele" defined with 12 atoms.
Mutagenesis: 5 rotamers loaded.
```

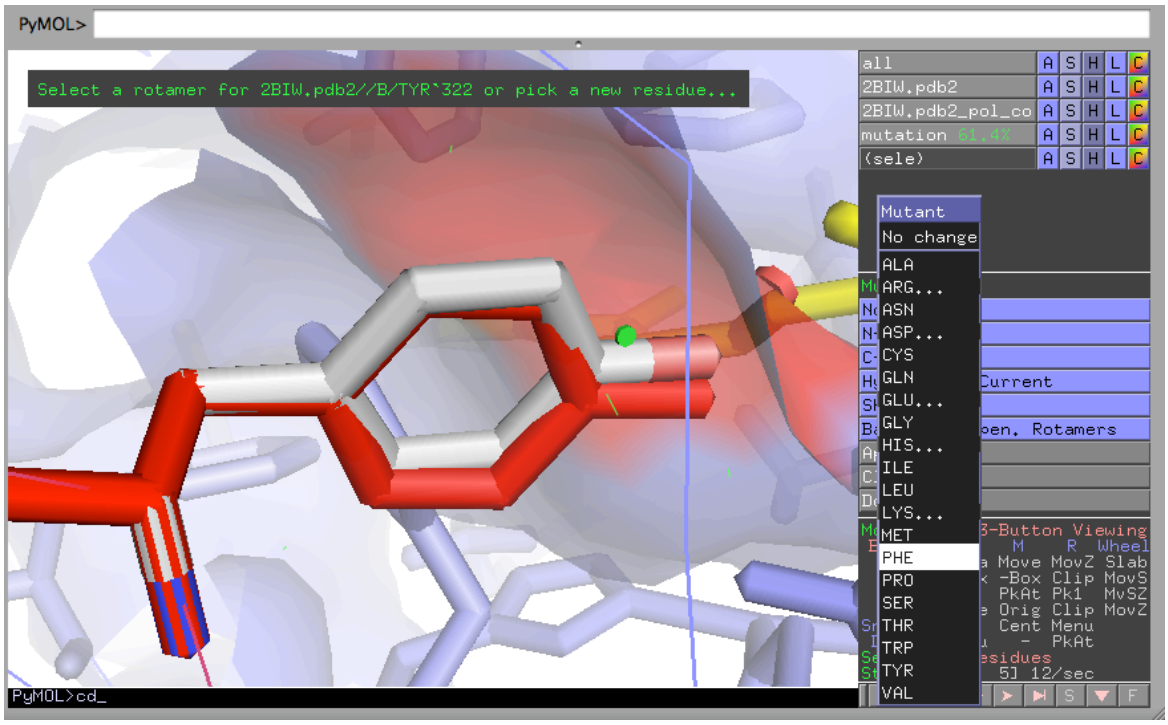
(Note: if Tyr 322 is still selected in (sele it may be necessary to click twice. The first click will unselect Tyr 322, and the second will select it for mutation.)

A new copy of Tyr322 will be displayed in white and corresponds to an ideal rotation. The default is that it is a backbone-dependent rotamer.

Upon selection a slight de-zooming may occur. Zoom back closer with the right-button mouse (Top > Down movement.)

- When "Select a rotamer for TYR`322 or pick a new residue…" appears at the top left: **Click on** the **white Tyr 322**

- **Click on** the **No Mutation button** and **select** a new amino acid : **PHE**



- **Click** the grey button **Apply**
- **Click** the grey button **Done**

Note: Clicking Done will exit the Mutagenesis Wizard.

✔ TASK

√ - Quit PyMol

---

12 *PyMol - Exercise L*: Model Building, helix modeling example

✔ READ

PyMol offers modeling options for small molecules and proteins. For example you can build an alpha helix from scratch with a specific sequence.

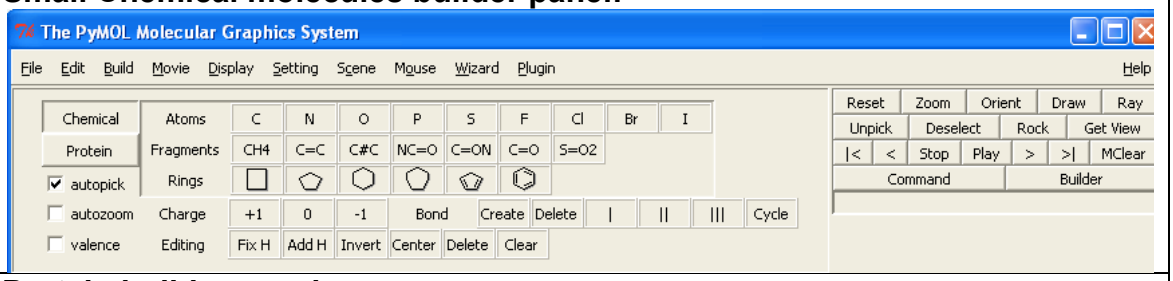
The “builder” interface to accomplish this is different depending on the operating system.

On Windows and X11 (Unix/Linux) versions of PyMol, the “External GUI” has an extra set of buttons to build by clicking on the various components to be assembled such as amino acids.

The MacPyMol version has the same capability but instead of clicking icons menu items are chosen.

Windows builder interface:

Small Chemical molecules builder panel:

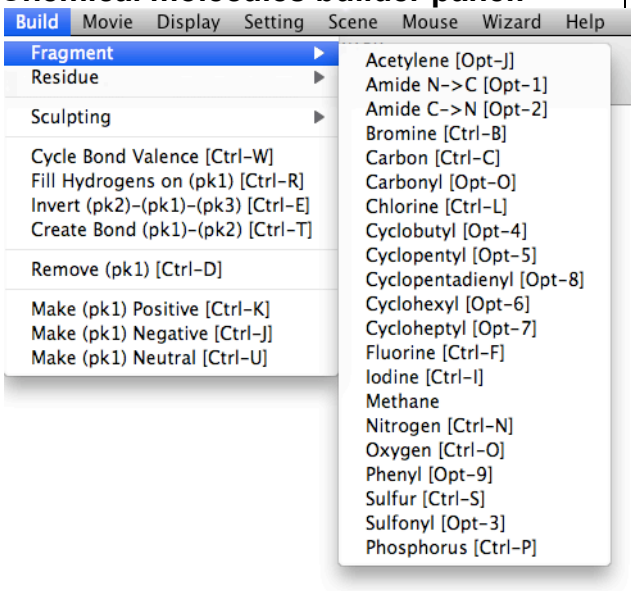

The PyMOL Molecular Graphics System
File Edit Build Movie Display Setting Scene Mouse Wizard Plugin Help
Chemical Protein autopick autozoom valence
Atoms C N O P S F Cl Br I
Fragments CH4 C=C C#C NC=O C=ON C=O S=O2
Rings
Charge +1 0 -1 Bond Create Delete | || ||| Cycle
Editing Fix H Add H Invert Center Delete Clear
Reset Zoom Orient Draw Ray
Unpick Deselect Rock Get View
|< < Stop Play > >| MClear
Command Builder

Protein builder panel:

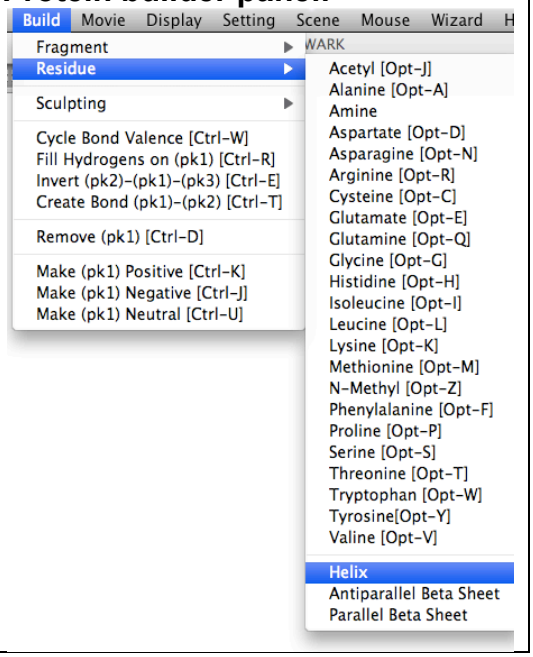
Chemical Protein autopick autozoom valence
Ala Asp Asn Arg Cys Glu Gln Gly His Ile Leu Lys
Met Phe Pro Ser Thr Trp Tyr Val Ace NMe
Secondary Structure: Next... parallel beta sheet
Charge +1 0 -1 Bond Create Delete | || ||| Cycle
Editing Fix H Add H Invert Center Delete Clear
Reset Zoom Orient Draw Ray
Unpick Deselect Rock Get View
|< < Stop Play > >| MClear
Command Builder

MacPyMol builder interface: **is via the Build menus:**

Chemical molecules builder panel:



Protein builder panel:



INFO

MacPyMol is a hybrid version that also contains the X11 version. To access the X11 version simply copy and rename the MacPyMol application (e.g. on the Desktop) with the menu cascade:

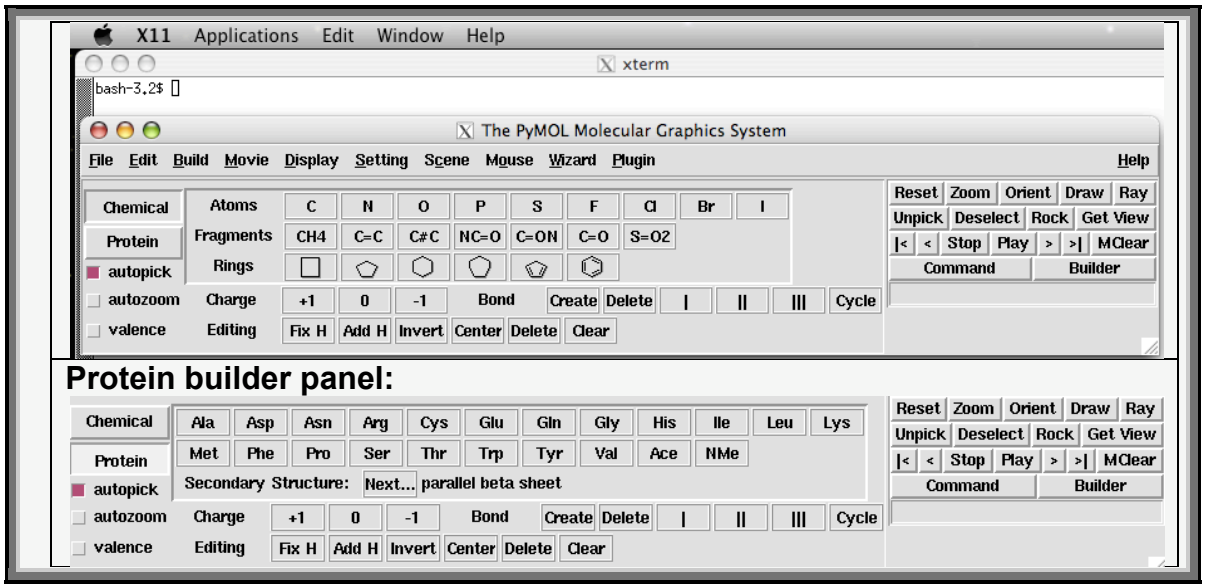
- √ - **Click once** on MacPyMol
- √ - use the Finder menu: **Edit > Copy**
- √ - **Click** anywhere on the **Desktop** , then **Edit > Paste**
- √ - **Change** the name from "**MacPyMol Copy**" to "**PyMOLX11Hybrid**"
- √ - The change of name will activate the X11 version embedded within upon double clicking

Note: X11 has to be installed on the Macintosh for this to work. Current versions of the Mac OS install X11 by default.
Note: an Xterm terminal will appear

The X11 version looks very similar to the Windows version, including a split between the external and internal GUIs.

X11 builder interface:

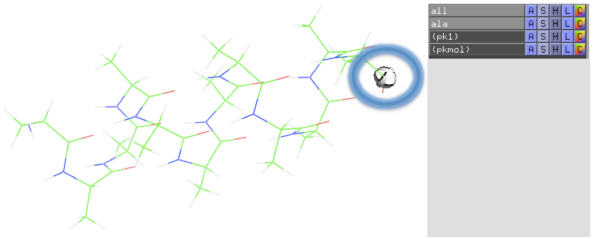
Small Chemical molecules builder panel:


X11 Applications Edit Window Help
xterm
bash-3.2$
The PyMOL Molecular Graphics System
File Edit Build Movie Display Setting Scene Mouse Wizard Plugin Help
Chemical
Protein
autopick
autozoom
valence
Atoms C N O P S F Cl Br I
Fragments CH4 C=C C#C NC=O C=ON C=O S=O2
Rings
Charge +1 0 -1
Editing Fix H Add H Invert Center Delete Clear
Bond Create Delete | || ||| Cycle
Reset Zoom Orient Draw Ray
Unpick Deselect Rock Get View
|< < Stop Play > >| MClear
Command Builder
Protein builder panel:
Ala Asp Asn Arg Cys Glu Gln Gly His Ile Leu Lys
Met Phe Pro Ser Thr Trp Tyr Val Ace NMe
Secondary Structure: Next... parallel beta sheet

12.1 Steps to build a poly-Alanine model helix:

a. Macintosh MacPyMol: follow the menu cascades:

b.

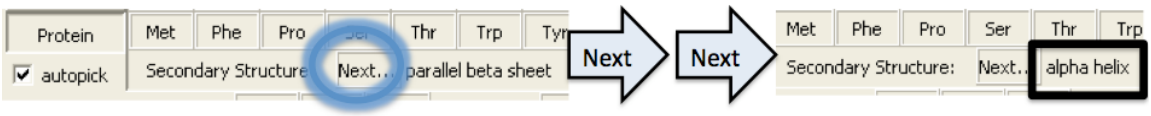


√ - **Build > Residue > Helix**
√ - **Build > Residue > Alanine**
√ - **Repeat** another 11 times for a total of 12 residues
√ - Alternatively use the **Option+A** keyboard shortcut
√ - The model will be built within the Viewer and have name “ala” within the Names Panel.

Note: the C carbon to which the next amino-acid is attached is shown by a spherical symbol.

c. Windows / X11:

√ - **Click** on “**Builder**” button (far right)
√ - **Click** on “**Protein**” button (far left)
√ - **Change** the **default** parallel-beta sheet to helix: bottom of menu: Click “next” twice



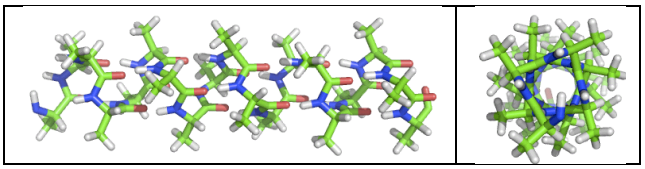
√ - **Click** on **Ala 12 times**

√ - The model will be built within the Viewer and have name “ala” within the Names Panel.

d. Save the molecule into a file:

√ - menu **File > Save Molecule** .
√ - verify that “ala” is selected, or click on ala.
√ - Click OK
√ - The default name is the name of the first amino acid used e.g. **ala**.pdb

The alpha helix is created as a “**perfect**” model and contains all hydrogen atoms.



13 *PyMol - Exercise M*: Displaying hydrogen bonds.

INFO
See also “Polar Contacts” within the following web page:
http://www.pymolwiki.org/index.php/Displaying_Biochemical_Properties

In the previous exercise we created a short α-helix, which we will use here for illustration.

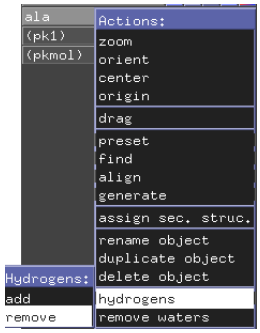
13.1 Example 1: short helix model

It will be easier to display and see the hydrogen bonds if the hydrogen atoms are removed:

TASK

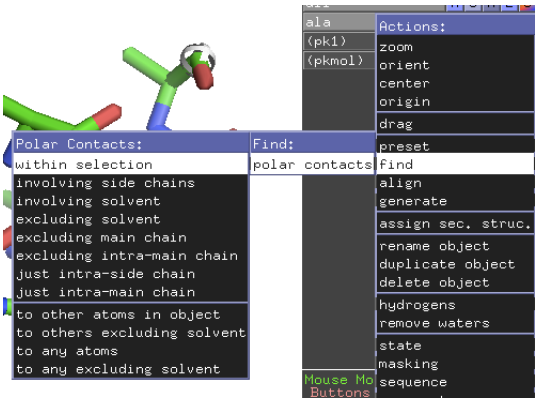
√ - Remove hydrogens with the menu cascade within the Names panel:

ala > A > hydrogens > remove

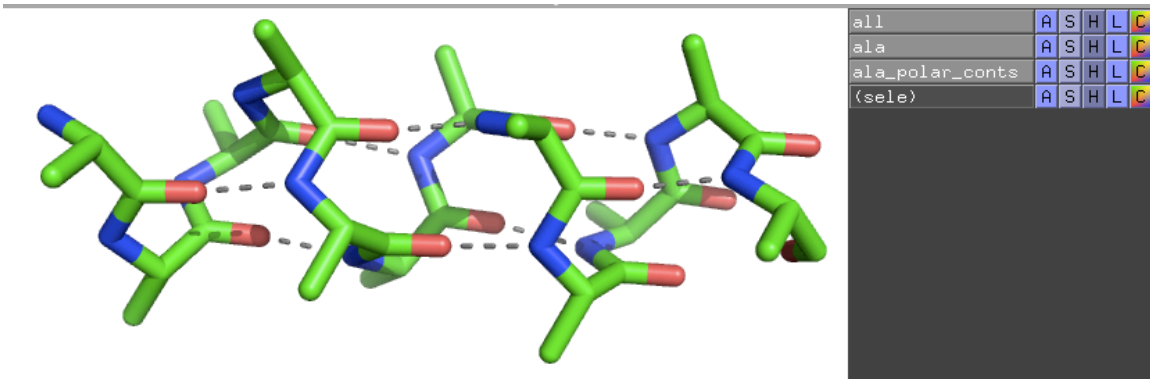


To display hydrogen bonds, follow the menu cascade from the Names panel:

ala > A > find > polar contacts > within selection



Note: the bonds are shown as yellow, dashed lines, which can be changed to a darker color with the C Names panel button.



Note: the polar contacts are created under the entry named **ala_polar_conts** within the Names panel and this button can be clicked to toggle the display of the bonds on and off.

√ **- Click** on **all** within the Names panel to render all displays invisible as a preparation for the next exercise below.

13.2 Example 2: helix segment within 2BIW.pdb2

✔ TASK

√ **- load** the **2BIW.pdb2** file (one more time!)
√ **-** Within the Names panel: **2BIW.pdb2 > H > everything**

The following is an example to display the hydrogen bonds within the alpha helix consisting of residues 94 to 105 in 2BIW.pdb2:

√ **-** First **create object "helix-1"** containing the helix residues by **typing the following line** within the line-command area (this type of command and its syntax will be reviewed in details in the next lab.)

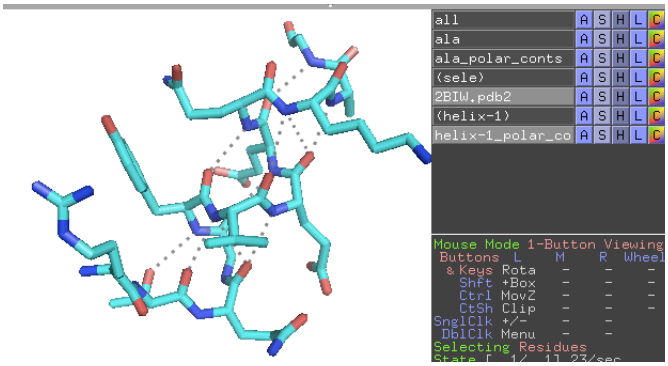
```
select helix-1, resi 94-105
```

√ **-** Display the selection (Names panel): **(helix-1) > S > sticks**

√ - For easier rotation enter the line-command: **center helix-1**
√ - Then find the polar contact the menu cascade from Names panel:

(helix-1) > A > find > polar contacts > within selection

A new objects **2BIW.pdb2_polar_conts** is created. The yellow default color for the dashed line is easily changed with the **C** menu for this object. For example a darker color can be chosen for display against a white background.



Note: choosing **to other atoms in object** would show additional hydrogen bonds of the helix side-chains to other parts of the protein.

Note: for more complex issues regarding hydrogen bonds or adding hydrogen atoms refer to the web link above.

PyMol continues with PyMol 2 L02 module.

Class notes